Semiclassical calculation of bound states of a multidimensional system*

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The semiclassical quantum conditions for bound states are studied for a nonseparable system of two coupled oscillators which possesses a collection of quasiperiodic trajectories. The semiclassical energy levels are found to be in excellent agreement with the exact quantum levels. This treatment differs from previous work in that periodic trajectories are not needed and in that the potential surface is smooth and nonseparable in all regions.

INTRODUCTION

The calculation of bound state properties within the semiclassical approximation for systems with more than one degree of freedom has attracted considerable attention for many years. In spite of this, there exists no practical semiclassical quantum condition which allows one to decide which classical states correspond to quantum mechanical bound states for general multidimensional systems unless the system happens to be separable. In the present work the quantum conditions are studied for a nonseparable, two dimensional system which possesses a collection of trajectories which generate a complete, multivalued solution of the Hamilton–Jacobi equation throughout a region of coordinate space. The energy levels computed from the quantum conditions for this system are then compared with the exact, numerically computed, quantum mechanical energy levels of the system.

Historically, the problem of finding the quantum conditions for a mechanical system was circumvented by the formulation of quantum mechanics. However, there remains interest in the problem in part because there exist many systems which can be treated by classical mechanics but which are intractable by quantum mechanical methods. Then such semiclassical quantum conditions would provide a way of extracting information about quantum mechanical bound states from the available classical mechanical data.

The approach in this study is most like that of Keller[1] in that it depends on the multivalued solutions of the Hamilton–Jacobi equation. In Keller's treatment, the quantization condition is derived from the requirement that the various branches of the semiclassical wavefunction connect properly along the caustic curves. The same quantum conditions were derived by Marcus[2] by requiring that the semiclassical wavefunction go over to an exponentially decreasing function at all points on the caustic curve. Keller and Rubinow[3] applied the theory to a free particle in two dimensions constrained by hard walls. In the system used in the present work the particle moves on a smooth potential in which the two degrees of freedom are coupled in all regions of the coordinate space.

Another approach to the semiclassical theory of bound states is that of Gutzwiller[4–7] and W. H. Miller[8] which is based on a semiclassical approximation to the quantum mechanical Green's function. Their result is that a system has a bound state at an energy if the classical system has, at this energy, a periodic trajectory which satisfies a quantum condition. In contrast, the existence of quantized periodic trajectories is neither necessary nor sufficient in the present treatment.

Pechukas[9] has extended to several dimensions the transformation of the Schrödinger equation used by S. C. Miller and Good[10] and has studied the class of multidimensional systems which result from a Miller–Good transformation of separable systems. The system studied in the present work has the qualitative features of the Miller–Good transformed systems, but the treatment here does not require one to find the Miller–Good transform or even to know if it exists. Pechukas[9] also gives a critical review of previous work on the semiclassical treatment of bound states.

In the next section the properties of the system are discussed, and the quantum conditions are exhibited. The last section contains the details of the method for computing the semiclassical energy levels of the system and the comparison with the quantum energy levels.

SEMICLASSICAL QUANTUM CONDITIONS

The Hamiltonian for the system to be considered here is given by

$$E = \tfrac{1}{2}(P_x^2 + P_y^2 + \omega_x^2 x^2 + \omega_y^2 y^2) + \lambda x(y^2 + \eta x^2) \,. \tag{1}$$

The coordinates are x and y; the corresponding momenta P_x and P_y; ω_x, ω_y, λ, and η are constants; and E is the total energy of the system. Physically this Hamiltonian represents a system of harmonic oscillators of unit mass with frequencies ω_x and ω_y coupled by a cubic potential, the strength of which is determined by λ and η. A Hamiltonian of this form might be obtained, for example, by transforming an anharmonic triatomic oscillator into some approximate normal mode coordinates, neglecting bending. Then the strength of the anharmonicity would determine λ and η. This system has been studied extensively in the past by workers in many fields.[11–14]

It has been shown by Kolmogorov, Arnold, and Moser[15] that many coupled, multidimensional systems possess quasiperiodic trajectories, by which it is meant that the coordinates and momenta may be expanded as functions of time in a convergent Fourier series with a finite number of fundamental frequencies. One result of this theorem is that such a system may be confined

to a region of coordinate space smaller than that allowed by the total energy of the system. One of the simplest of such systems is that of Eq. (1). A typical trajectory of this Hamiltonian is shown in Fig. 1. This trajectory fills a "box" with slightly curved sides *ABCD*, which is contained within the oval-shaped equipotential curve. The equipotential curve encloses the area in which the trajectory is confined by energy conservation and is the locus of points (x, y) satisfying

$$E = \tfrac{1}{2}(\omega_x^2 x^2 + \omega_y^2 y^2) + \lambda x(y^2 + \eta x^2) \ . \tag{2}$$

The trajectory touches the equipotential curve only at zero momentum, which is the case at the "corners" of the box *ABCD*. The "sides" or envelopes *AB*, *BC*, *CD*, and *DA* are called the caustic curves for the trajectory since they are the curves on which adjacent trajectories cross each other. The caustic curves are the analogs of the turning points in one dimension. It would appear from Fig. 1 that there exist no other such caustic curves.

For a trajectory such as that in Fig. 1, a multivalued pair of momentum functions $P_x(xy)$, $P_y(xy)$ may be defined by the equations

$$P_x(x(t),\ y(t)) = P_x(t)\,; \quad P_y(x(t),\ y(t)) = P_y(t) \ , \tag{3}$$

where $x(t)$, $y(t)$, $P_x(t)$, and $P_y(t)$ are the coordinates and momenta as functions of time t satisfying Hamilton's equations of motion corresponding to the Hamiltonian of Eq. (1). There are four branches of this pair of functions, since the trajectory may pass through a given point (x, y) moving in four different, general directions. The branches are distinguished by a superscript Roman numeral I, II, III, or IV depending on whether the trajectory which passes through the point (x, y) is moving in the general direction of the upper right, upper left, lower left, or lower right portion of Fig. 1, respectively. In Fig. 2 a portion of the trajectory of Fig. 1 is shown along with the Roman numeral denoting the branch of the momentum function generated by the trajectory between successive points where it touches the caustic curve.

The fact that only four such branches of $P_x(xy)$, $P_y(xy)$ exist and are well defined over the same region of the x–y plane is a consequence of the assumption that there are four well defined caustic curves as shown in Fig. 1. Studies of the system of Eq. (1) have indicated that most of the trajectories at the energies where the system has bound states have these properties.[16] Exceptions to this statement occur for trajectories in which most of the energy is in one degree of freedom,[16] for systems in which the frequencies ω_x and ω_y are equal,[17] and in certain other systems[11] at high total energy E or with large values of the coupling parameters λ and η. In these exceptional cases the trajectories may fill a more complicated region[11] or may appear to be ergodic and not be confined to any region smaller than that allowed by the conservation of energy. For such systems other methods than those described here would be needed and are under investigation.

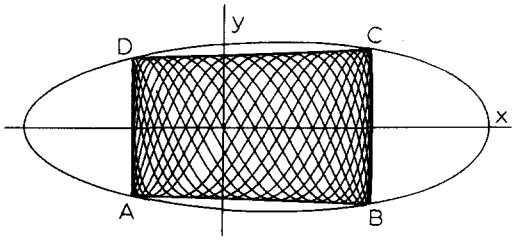

FIG. 1. A typical trajectory of the coupled, two dimensional system considered in this work, having the Hamiltonian of Eq. (1). The trajectory appears to stay forever within the "box" *ABCD* rather than wandering throughout the energetically allowed region within the oval-shaped curve. This particular trajectory has frequencies such that $\omega_x^2 = 0.29375$, $\omega_y^2 = 2.12581$; coupling parameters $\lambda = -0.1116$, $\eta = 0.08414$; and is initially at the origin with positive momenta determined by the total energy, $E = 2.42$, and fraction of energy in the x oscillator, $f_x = 0.25$, cf., Eq. (18).

A multivalued solution of the Hamilton–Jacobi equation may be written in terms of the momentum functions $P_x(xy)$, $P_y(xy)$. The Hamilton–Jacobi equation corresponding to Eq. (1) is

$$\frac{1}{2}\left[\left(\frac{\partial\Phi(xy)}{\partial x}\right)^2 + \left(\frac{\partial\Phi(xy)}{\partial y}\right)^2 + \omega_x^2 x^2 + \omega_y^2 y^2\right] + \lambda x(y^2 + \eta x^2) = E \ . \tag{4}$$

Solutions of Eq. (4) are well known to be[18,19]

$$\Phi^\gamma(xy) = \Phi^\gamma(x_0 y_0) + \int_{x_0 y_0}^{xy} [P_x^\gamma(x'y')\,dx' + P_y^\gamma(x'y')\,dy'] \ ,$$
$$\gamma = \mathrm{I},\ \mathrm{II},\ \mathrm{III},\ \mathrm{IV} \ , \tag{5}$$

where the point (x_0, y_0) and the value $\Phi^\gamma(x_0 y_0)$ at that point are arbitrary. Here γ indicates the branch I, II, III, or IV of the functions $P_x(xy)$ and $P_y(xy)$ and therefore of the multivalued function $\Phi(xy)$. The integral in Eq. (5) is a line integral and may be shown to be independent of path.

Action variables J_x and J_y, which are constants of the motion along the trajactory, are defined by

$$J_x = \int_l^r [P_x^{\mathrm{I}}(xy)\,dx + P_y^{\mathrm{I}}(xy)\,dy] + \int_r^l [P_x^{\mathrm{II}}(xy)\,dx + P_y^{\mathrm{II}}(xy)\,dy] \ ,$$
$$J_y = \int_b^u [P_x^{\mathrm{I}}(xy)\,dx + P_y^{\mathrm{I}}(xy)\,dy] + \int_u^b [P_x^{\mathrm{IV}}(xy)\,dx + P_y^{\mathrm{IV}}(xy)\,dy] \ . \tag{6}$$

Here l is a point on the left caustic curve *AD* of Fig. 1, r is a point on the right caustic *BC*, b is on the lower caustic *AB*, and u is on the upper caustic *CD*. Since the line integrals in Eqs. (6) are independent of path, it may be shown that J_x and J_y are independent of the location of the points l, r, b, and u as long as the points are on the indicated caustic curve.

So far only one trajectory has been considered. Other trajectories of the type shown in Fig. 1 will generate other multivalued solutions $\Phi(xy)$ and define different action variables J_x, J_y by Eqs. (6). For example, if the

collection of trajectories with initial conditions $x(0)=x_0$, $y(0)=y_0$ for some x_0, y_0 are considered, there will exist a multivalued solution $\Phi(x\,y)$ and J_x, J_y for each different set of initial momenta $P_x(0)$, $P_y(0)$ provided the trajectories are of the type pictured in Fig. 1. The trajectories may as well be considered to be indexed by the action variables J_x, J_y so that Φ may also be considered to be a function of these constants. The multivalued solution $\Phi(x\,y\,J_x J_y)$ of the Hamilton–Jacobi Eq. (4) is a complete solution in the sense that it is a solution containing two arbitrary constants, J_x and J_y.[18,19] Therefore $\Phi(x\,y\,J_x J_y)$ generates a canonical transformation from coordinates x, y and momenta P_x, P_y to new momenta (action variables) J_x, J_y and new coordinates (angle variables) w_x, w_y defined by the equations

$$P_x=\frac{\partial\Phi(x\,y\,J_x J_y)}{\partial x}\,;\quad P_y=\frac{\partial\Phi(x\,y\,J_x J_y)}{\partial y}\,;$$
$$w_x=\frac{\partial\Phi(x\,y\,J_x J_y)}{\partial J_x}\,;\quad w_y=\frac{\partial\Phi(x\,y\,J_x J_y)}{\partial J_y}\,. \tag{7}$$

The new Hamiltonian is just the old Hamiltonian, Eq. (1), expressed in terms of the new coordinates and momenta and is a function of the new momenta J_x, J_y only, since they are constants of the motion. Therefore the angle variables w_x, w_y are linear functions of time.

The quantum conditions for the system are[1,2]

$$J_x=2\pi(n_x+\tfrac{1}{2})\hbar\,;\quad J_y=2\pi(n_y+\tfrac{1}{2})\hbar\,, \tag{8}$$

where n_x and n_y are positive integers. That is, an energy E is an allowed energy level of the system if there exists a classical trajectory at that energy of the type in Fig. 1 defining action variables satisfying Eqs. (8). In what follows it will be convenient to define continuous quantum numbers n_x and n_y for every J_x and J_y by Eqs. (8). If the classical Hamiltonian in action-angle variables is

$$H(J_x,\,J_y)=E\,, \tag{9}$$

then the total energy E may be considered to be a function of n_x, n_y thus:

$$E(n_x n_y)=H(2\pi(n_x+\tfrac{1}{2})\hbar\,,\quad 2\pi(n_y+\tfrac{1}{2})\hbar)\,. \tag{10}$$

Therefore, an equivalent statement of the quantum conditions is that $E=E(n_x n_y)$ is an allowed energy of the system if both n_x and n_y are integers.

These quantum conditions may be derived or rationalized in a variety of ways. In the old quantum theory, for example, the restriction of Eqs. (8) is a matter of hypothesis,[20] except that in most nonseparable, multidimensional systems it is difficult to define unique action variables. The present system is an example of one in which action variables may be defined as previously discussed.

The quantum conditions (8) may be justified in an intuitive manner by solving the semiclassical Schrödinger equation in action-angle variables. The semiclassical Schrödinger equation is obtained from Eq. (9) by the use of the approximate, semiclassical prescription[21–23]

$$J_x=\hbar/i\,\partial/\partial w_x+\pi\hbar\,;\quad J_y=\hbar/i\,\partial/\partial w_y+\pi\hbar \tag{11}$$

to be

$$H(\hbar/i\,\partial/\partial w_x+\pi\hbar\,,\ \hbar/i\,\partial/\partial w_y+\pi\hbar)\Psi(w_x w_y)$$
$$=E\Psi(w_x w_y)\,, \tag{12}$$

where $\Psi(w_x w_y)$ is the wavefunction. The substitution of Eqs. (11) is correct only within the semiclassical approximation.[23] In Eqs. (11), the term $\pi\hbar$ has been added to the well known prescription of Dirac[21,22] and others in order that the prescription give the quantum conditions which are known to be correct for the special case of a separable system of independent oscillators. A solution of Eq. (12) is[24]

$$\Psi(w_x w_y)=\exp[2\pi i(n_x w_x+n_y w_y)] \tag{13}$$

where n_x and n_y are constants. It is a property of the transformation generated by $\Phi(x\,y\,J_x J_y)$ by Eqs. (7) that the mapping is periodic with unit period in each of the angle variables w_x and w_y.[18,19] For example, both of the points (w_x, w_y, J_x, J_y) and (w_x+1, w_y, J_x, J_y) in the phase space of action-angle variables represent the same point in the phase space of the old coordinates and momenta. In order to be single valued, $\Psi(w_x w_y)$ must be periodic in w_x and w_y and thus the constants n_x and n_y must be integers. The energy levels are obtained by the substitution of Eq. (13) into Eq. (12) with the result

$$H(2\pi(n_x+\tfrac{1}{2})\hbar\,,\quad 2\pi(n_y+\tfrac{1}{2})\hbar)\Psi(w_x w_y)=E\Psi(w_x w_y)\,, \tag{14}$$

which is equivalent to Eq. (10). The constants n_x, n_y are seen to be the same as those in Eqs. (8).

The same quantum conditions have also been derived by Keller[1] by requiring that the semiclassical wavefunction be single valued in the x–y coordinates and making use of a phase integral method. An intuitive view of the appearance of the half-integers in Eq. (8) is provided by the effect of the turning points of each vibration on the phase of the semiclassical wavefunction.[1] Each turning point reflects the wave, causing a phase loss of $\pi/2$ per reflection, and two reflections occur in one complete period. The quantum conditions have also been obtained by Marcus[2] as discussed in the last section. The treatment of Marcus makes use of an approximate separation of variables in the vicinity of each point on the caustic curve to match the semiclassical wavefunction in the classically allowed region to a function which vanishes asymptotically.

CALCULATIONS

In general terms, the semiclassical calculation of the energy levels of the system of Eq. (1) was carried out by computing J_x and J_y from the definitions (6) using trajectory data computed numerically. The calculation was repeated for different trajectories until J_x and J_y were obtained satisfying the quantum conditions (8).

In principle any path between the left and right caustic curves of Figs. 1 and 2 would be suitable for the computation of J_x, for example, by Eqs. (6). But in practice it was found most convenient to use a path along the lower or upper caustic curve AB or CD of Fig. 1. The reason for this choice is that once the location of the

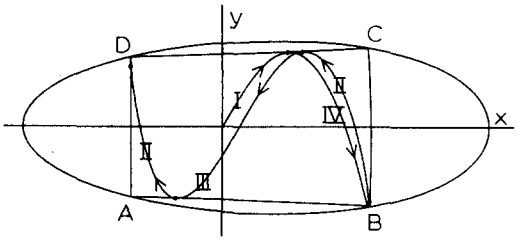

FIG. 2. A portion of the trajectory of Fig. 1 with the four branches of the momentum functions $P_x(xy)$, $P_y(xy)$ generated by it marked. The dots indicate the points where the trajectory touches the caustic curves, which are the nearly straight lines forming the sides of the "box" *ABCD*.

caustic curve is known from numerical trajectory data, the momenta P_x and P_y at each point on the curve are known from the Hamiltonian and the total energy of the system. More precisely, if x, y are the coordinates of a point on the lower caustic curve AB, then the momentum of the trajectory at the time when it touches AB at (x, y) is tangent to AB at (x, y). Thus, the components P_x, P_y of the momentum at the point (x, y) are related by

$$P_y/P_x = m(xy) , \tag{15}$$

where $m(xy)$ is the slope of AB at (x, y). If Eq. (15) is solved for P_y and is substituted into the Hamiltonian Eq. (1), the result for P_x and P_y is

$$P_x(xy) = \pm\{[2E - \omega_x^2 x^2 - \omega_y^2 y^2 - 2\lambda x(y^2 + \eta x^2)]/ [1 + m(xy)^2]\}^{1/2} , \tag{16}$$

$$P_y(xy) = m(xy)\, P_x(xy) .$$

The solution with the positive square root yields the momenta on branch I and the negative root yields branch II. Since the values of the momenta on the two branches have the same magnitude along AB, the expression for J_x from Eqs. (6) reduces to

$$J_x = 2\int_A^B [|P_x(xy)|\,dx + |P_y(xy)|\,dy] \tag{17}$$

with $P_x(xy)$, $P_y(xy)$ given by Eqs. (16). A similar expression is obtained for J_y.

The computation was carried out with a program written in FORTRAN for an IBM 360 Model 75 digital computer. The details of the calculation are as follows. For simplicity only the integration along the lower caustic curve AB of Fig. 1 is described since the calculation for another caustic is similar. Initial conditions for a trajectory are chosen to be $x(0) = 0$, $y(0) = 0$, and positive $P_x(0)$ and $P_y(0)$ determined by the specification of the total energy E and f_x, the fraction of energy initially in the "x oscillator." That is

$$f_x = P_x(0)^2/[P_x(0)^2 + P_y(0)^2] . \tag{18}$$

The trajectory is computed by solving Hamilton's equations for Eq. (1) by a Hamming predictor-corrector method. In the vicinity of each lower turning point where $P_y(t)$ has a zero and $y(t)$ is negative, y is approximated as a quadratic function of x. After the trajectory has been computed to such an extent as to clearly define the caustic curve, the points on the caustic curve are computed to be those points where a straight line is tangent to the quadratic approximation to the trajectory in the vicinity of two adjacent turning points. The computed points nearest the corners A and B are linearly extrapolated to the corners by using the fact that the coordinates of the points A and B satisfy Eq. (2). Finally the integral in Eq. (17) is performed numerically down straight line segments joining the points on the caustic curve just computed using Simpson's rule in each segment. In each segment the momenta $P_x(xy)$ and $P_y(xy)$ in the integrand of Eq. (17) are given by Eqs. (16).

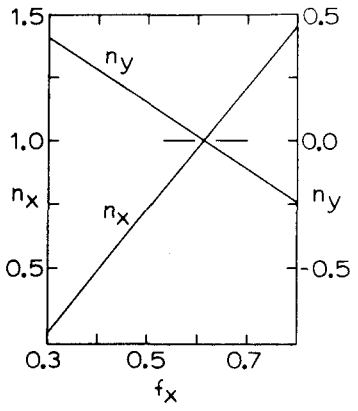

FIG. 3. The quantum numbers n_x and n_y computed from various trajectories. All of the trajectories have the same total energy $E = 1.6870$ and differ in f_x, the energy initially in the x oscillator. This total energy is clearly a semiclassically allowed energy level of the system since both n_x and n_y are integers at $f_x = 0.6120$. The system has the Hamiltonian of Eq. (1) with frequencies such that $\omega_x^2 = 0.49$, $\omega_y^2 = 1.69$ and coupling parameters $\lambda = -0.1$, $\eta = 0.1$.

It may be seen that the above procedure will yield the actions J_x and J_y or, by Eqs. (8), the quantum numbers n_x and n_y to any desired accuracy provided a sufficient number of points on the trajectory are computed to high enough accuracy and enough steps are taken in the numerical integration of Eq. (17) and provided that the caustic curve is not too severely slanted. Tests have shown that the method is entirely adequate for the system studied here.

In Fig. 3 the quantum numbers n_x and n_y are plotted as a function of the fraction of the energy initially in the x oscillator, f_x, at a single total energy E. The two

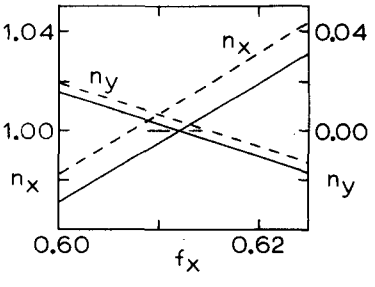

FIG. 4. Enlarged drawing of Fig. 3. The dashed line shows n_x and n_y for $E = 1.7000$ which is the energy level for the uncoupled system having $\lambda = 0$, cf., Eq. (1). The shift in the $n_x = 1$, $n_y = 0$ energy level due to the coupling for the nonzero λ is clearly seen.

TABLE I. Comparison of the semiclassical and quantum energy levels for various systems.

System[a]				Quantum numbers			$E(n_x n_y)$	Uncoupled
ω_x^2	ω_y^2	λ	η	n_x	n_y	Quantum	Semiclassical	$\lambda=0$
0.29375	2.12581	−0.1116	0.08414	0	0	0.9916	0.9920	1.0000
				1	0	1.5159	1.5164	1.5420
				2	0	2.0308	2.0313	2.0840
				0	1	2.4188	2.4196	2.4580
0.36	1.96	−0.1	0.1	0	0	0.9939	0.9942	1.0000
				1	0	1.5809	1.5813	1.6000
				2	0	2.1612	2.1615	2.2000
0.49	1.69	−0.1	0.1	0	0	0.9955	0.9955	1.0000
				1	0	1.6870	1.6870	1.7000
				0	1	2.2781	2.2780	2.3000
				2	0	2.3750	2.3750	2.4000
				1	1	2.9583	2.9584	3.0000
0.81	1.21	−0.08	0.1	0	0	0.9980	0.9978	1.0000
				1	0	1.8944	1.8941	1.9000
				0	1	2.0890	2.0897	2.1000
				2	0	2.7899	2.7895	2.8000

[a]Parameters of Eq. (1).

constants E and f_x determine a trajectory with the indicated values of n_x and n_y. The total energy considered in Fig. 3 is a semiclassical energy level of the system since n_x and n_y are simultaneously integers for $f_x = 0.6120$. The same data are plotted on an expanded scale in solid lines in Fig. 4. Also shown in dashed lines are the n_x and n_y computed at a higher energy which would be an energy level of the system in the absence of the coupling term in Eq. (1), i.e., if $\lambda = 0$. It may be clearly seen from Fig. 4 that the cubic coupling due to nonzero λ has shifted the energy level.

In order to compute the semiclassical energy levels, $E(n_x n_y)$ of Eq. (10) with integer n_x and n_y, the values of n_x and n_y were computed for three different trajectories corresponding to different values of the pair E, f_x. These data were used in an interpolation scheme to be described presently to obtain an estimate of the E, f_x which would yield the desired integer values of n_x and n_y. The values of n_x, n_y actually computed from this last estimated E, f_x were used in the interpolation scheme together with the data from the previous two trajectories to obtain a better estimate of E, f_x. This procedure was repeated until E was obtained to the desired accuracy. Generally only one or two iterations, which is a total of four or five trajectories, were required to obtain an energy level to the five significant figures reported in this work.

The interpolation precedure makes use of the fact that n_x and n_y are nearly linear functions of f_x and E as is partially evident from Figs. 3 and 4. Values of n_x and n_y from three different trajectories were fitted to expressions of the form

$$n_x = a_x E + b_x f_x + c_x \; ; \quad n_y = a_y E + b_y f_x + c_y \, , \tag{19}$$

and the constants a_x, b_x, c_x, a_y, b_y, and c_y were determined. Then the desired integer n_x and n_y were inserted into Eqs. (19) and the resulting pair solved for the new estimate of E and f_x.

In order to compare with these semiclassical results, the exact, quantum mechanical energy levels of the system of Eq. (1) were computed numerically. The wavefunction of the system was expanded in the set of eigenfunctions of the uncoupled system, which is the system having the classical Hamiltonian of Eq. (1) with $\lambda = 0$. Substitution of this expansion into the Schrödinger equation corresponding to the Hamiltonian of Eq. (1) leads to the usual algebraic eigenvalue problem, which was solved by standard numerical methods.[25]

All calculations reported here were carried out on the system given by Eq. (1) with units chosen such that

$$\hbar = 1 \text{ and } \omega_x + \omega_y = 2 \, . \tag{20}$$

One consequence of this choice of units is that the ground state of the uncoupled system ($\lambda = 0$) is at $E = 1$.

In Table I some of the semiclassical energy levels computed as described above are compared with the exact quantum results for various systems and coupling strengths. The first system in Table I, expressed in other units, is a system which has been studied in the past by several workers[26–28] from a purely classical point of view. Care was taken to insure that all of the energy levels were computed accurately to ±1 in the least significant figure reported.

It may be seen in Table I that the agreement between the semiclassical and quantum energy levels is excellent throughout, being generally better than ±4 in the fourth decimal place.

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